FACTORS AFFECTING THE THERMAL EFFICIENCY OF A GASIFICATION PROCESS

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Abstract - Two main factors affecting the thermal efficiency of the gasification process are the amount of methane formed in the gasifier and the kind of coal used. Thermal efficiencies are calculated for the various coal gasification processes having potential for commercialization. Another way of comparing different processes, based on the second law of thermodynamics considerations in terms of available work is introduced.

The results show that higher amounts of methane formed by direct methanation in the gasifier will result in higher thermal efficiency of the process. Thermal efficiency of Lurgi Process decreases considerably when higher ranking coals are used. The available work efficiency can be used not only for comparison but also to pinpoint inefficiencies inherent in certain process steps.

Introduction

Coal gasification processes for production of SNG can be divided into several individual sub-systems, such as coal preparation, pretreatment gasification, shift conversion, gas purification and methanation which may be followed by compression to desired pipeline gas pressure if necessary. As the products of gasification affect the overall thermal efficiency of the process greatly, gasification sub-system is described briefly in the following section.

Gasification

In gasification, coal is converted into gases that can be converted later into a pipeline quality gas having a heating value of more than 900 Btu/SCF. In a gasifier, following reactions take place:

$$\text{Coal} \xrightarrow{\text{Pyrolysis}} \text{Char} + \alpha CH_4 + \beta C_2H_6 + \gamma CO + \delta H_2 + \text{Moisture}$$

$$\text{Char} + \text{Steam} \rightarrow CO + H_2 \qquad 1)$$

$$CO + \text{Steam} \rightleftarrows CO_2 + H_2 \qquad 2)$$

$$\text{Char} + 2H_2 \rightarrow CH_4 \qquad 3)$$

Steam-char reaction is highly endothermic while water gas and hydrogasification reactions are exothermic. Heat required in reaction 1) can be supplied directly by coal-oxidation or indirectly by heating. (13)

The major factor affecting the thermal efficiency is the amount of methane formed in the gasifier. Amount of methane produced depends on pressure, temperature and the kind of gasifier used.

Effect of Methane Concentration in Gas from Gasifier on the Thermal Efficiency of the Process:

In Figure 1, heating value of the gas at the gasifier exit is plotted against the calculated values of overall thermal efficiency for various processes (2), (6). The results clearly show that when the amount of methane produced in the gasifier is higher, the thermal efficiency of the process is consistently higher. The reason for this is that the amount of hydrogen required to produce methane is less if hydrogen reacts with carbon in coal rather than with carbon in carbon monoxide or dioxide as it occurs in methanator later on. Also the heat generated in the gasifier because of hydrogasification reaction can be utilized to carry out the carbon-steam endothermic reaction in the gasifier. This heat utilization is more efficient than utilization of heat recovered in the form of high pressure steam in methanation. In addition, heat generated due to hydrogasification reaction reduces the oxygen requirements reducing the consumption of energy in the oxygen plant. Coal contains certain amounts of aliphatic compounds and hydrogen in the form of volatile matter. This volatile matter decomposes into low hydrocarbon compounds such as methane, ethane, etc., by reacting with hydrogen during the pyrolysis and the initial stage of gasification. For example, in Lurgi Process using moving bed gasifier, coal and gas flows are countercurrent and hence, large amounts of hydrogen is contacted with coal in the devolatilization zone (top of the reactor) producing methane.

Effect of Temperature and Pressure on Methane Production:

Amount of methane produced decreases with increase in temperature, e.g., in Koppers-Totzek Process, due to high temperature (3200°F) very little methane is produced (3). And, therefore, intensive methanation is required. However, due to high temperature, tar and higher hydrocarbons decomposes into carbon monoxide and hydrogen eliminating complications in the purification section found in other lower temperature processes. Amount of methane produced increases with the increase in pressure. This increase in methane concentration continues at pressures above 400 psig. (used in Lurgi gasifiers) and quantitative data on this phenomenon have been reported by B.C.R.(4).

The other factor affecting the thermal efficiency is the kind of coal gasified. Coal can be classified into peat, lignite, sub-bituminous, bituminous, semi-bituminous and anthracite. Lignite and sub-bituminous coals are usually caking coals and form non-porous coke on heating.

Effect of Coal on the Efficiency of the Gasification Process:

In coal-steam reaction, theoretically the following two forms of reactions can take place.

$$\text{Coal} + \text{Steam} \underset{\Delta H_R}{\rightarrow} CO + H_2 + CO_2 + H_2S \qquad 4)$$

$$\text{Coal} + \text{Steam} \underset{\Delta H_R}{\rightarrow} CO_2 + CH_4 + H_2S \qquad 5)$$

Even though reaction 4 and 5 are extremes, they take place simultaneously in a gasifier with few exceptions. For example, in Koppers-Totzek gasifier only reaction 4 occurs while in Hydrane gasifier reaction 5 occurs to large extent. Both of the above reactions are endothermic. Endothermicity of the reaction represents the amount of heat required to complete the reaction and in gasification, this heat is supplied by oxidation of coal with oxygen. The endothermicity of the reaction is different for different coal and since heat is supplied by oxidation of coal, it may be expected to be directly related to the efficiency of the process.

For three different coals, data shown in Table 1 were reported by Koppers company (3). These data show that the amount of oxygen and steam required for gasification increases with the increase in volatile matter. The data also show that the composition and the heating value of the gasifier product are almost similar in all cases and thus are nearly independent of kind of coal used. Carbon conversion is a function of reactivity of coal. Lignite and sub-bituminous coals can be converted almost completely while conversion of high volatile coals approaches 95%-97% (3). The same kind of data collected from trials at Westfield, Scotland, were reported by Lurgi for Montana, Illinois 5, Illinois 6 and Pittsburgh 8 coals.(1),(11)

TABLE 1 Effect of Coal on Gasifier Products, Koppers-Totzek Process (3)

Coal	Sub-bituminous Western	High Volatile B-Bituminous Illinois	High Volatile A-Bituminous Eastern
Composition (wt. %)			
C	56.76	61.94	69.88
H	4.24	4.36	4.90
O	13.18	6.73	7.05
N	1.01	0.97	1.37
S	0.67	4.88	1.08
Ash	22.14	19.12	13.72
Moisture	2.00	2.00	2.00
Heating Value BTU/lb.	9,888.	11,388.	12,696.
Gasification			
Oxygen required T/T of coal	0.649	0.704	0.817
Steam required T/T of coal	0.136	0.27	0.294
Gas Composition Dry Basis (Vol %)			
CO	58.68	55.38	55.90
CO_2	7.04	7.04	7.18
H_2	32.86	34.62	35.39
N_2	1.12	1.01	1.14
H_2S	0.28	.1.83	0.35
COS	0.02	0.12	0.04
	100.00	100.00	100.00
Gas Heating value BTU/SCF	295.1	290.2	294.4
No. of moles/ton of coal	136.4	156.6	174.8
Efficiency %			
Heating value of gas/ Heating value of coal	77.3	75.8	77.0
Heating value of gas/ Heating value of coal + + coal used for production of steam and power required.	69.7	67.9	68.7

These data are shown in Table 2. It can be concluded that higher operating temperature is necessary with decreasing coal reactivity. Oxygen and steam consumptions increase with the decrease in coal rank. However, yield of methane remains fairly constant for different kinds of coal. It also shows that efficiency of gasification, allowing for the coal equivalent of steam and oxygen supplies, decreases substantially with the increase in coal rank.

The type of coal processes also affects the amount of water required in a gasification process. The factors affecting the water requirements are:

a) Moisture content
b) Reactivity of coal
and c) Sulfur content of coal.

For a plant producing 250 MMSCF of pipeline gas, the total water requirement is roughly about 19,000 gpm. when lignite coal is used while for bituminous coal water required is about 22,500 gpm.

Thermal efficiency calculations done on the basis of first law of thermodynamics are useful for comparison of coal gasification processes. Another way of comparing different alternatives is to calculate energy utilization efficiency based on the second law of thermodynamics, which is defined as the ratio of total output of work equivalent in all outgoing streams to the total input. The main advantage of this approach is its ability to compare energy utilization efficiency of different processing schemes and alternatives, which may start from different energy resources and may produce different products, in a consistent way. It also pinpoints the inefficiencies inherent in certain process steps.

From second law of thermodynamics, the available work, $d\varepsilon$, can be expressed in terms of enthalpy change (dH) and entropy change (ds) as:

$$d\varepsilon = dH - T_o ds$$

where T_o is the temperature of the surrounding.

For a closed system in equilibrium at T_o, when no work can be obtained from it in the given surroundings,

$$\varepsilon = H - H_o - T(S-S_o)$$

is the maximum amount of work which can become available from the system if it can exchange heat only with a heat reservoir at T_o. A process stream carrying $\mathring{n}$ moles of i per unit of time and performing work $\mathring{w}$ in the same time is equivalent to a flux of available work

$$\mathring{\varepsilon} = \Sigma \mathring{n}_i \varepsilon_i + \mathring{w}$$

At steady state, for any system, the available work $\mathring{\varepsilon}_{in}$ entering the system is always greater than or equal to that leaving the system.

$$\mathring{\varepsilon}_{in} \geq \mathring{\varepsilon}_{out}$$

Then, the available work efficiency η can be defined as

$$\eta = \mathring{\varepsilon}_{out}/\mathring{\varepsilon}_{in}$$

The fraction $(1-\eta)$ is being lost due to irreversible processes causing an entropy production σ

$$(1-\eta)\ \overset{o}{\varepsilon}_{in} = T_o\ \sigma = I$$

Where I is the irreversible work associated with the entropy change.

The datum level used in available work efficiency calculations, is defined as one in which an existing substance, when in equilibirum with the surrounding, will have zero available work.

The bases used for calculations are air and water at 1 atm. and 25°C. Under these conditions, it may be assumed that available work from CO_2 and SO_2 is zero.

Table 2 Effect of coal on Gasifier Products
Lurgi Process (1)

Coal	Rosebud Montana	Illinois #5	Illinois #6	Pittsburgh #8
Composition wt %				
C	50.56	64.11	64.16	74.15
H	3.18	4.36	4.34	5.04
O	9.80	7.04	8.10	4.52
N	0.91	1.22	1.21	1.35
S	1.09	3.13	2.80	2.52
Ash	9.76	8.20	9.16	7.84
Moisture	24.70	11.94	10.23	4.58
	100.00	100.00	100.00	100.00
Heating value Btu/lb	8611.	11456.	11464.	13442.
Gasification				
Oxygen required T/T of coal	0.24	0.46	0.45	0.59
Steam required T/T of coal	1.25	2.25	2.51	3.24
Gas composition Dry Basis (%)				
CO	15.1	17.6	17.3	16.9
CO_2	30.4	31.0	31.2	31.5
H_2	41.1	38.8	39.1	39.4
N_2	1.2	1.5	1.2	1.6
H_2S	0.5	1.1	1.1	0.8
CH_4	11.2	9.2	9.4	9.0
C_2H_6	0.5	0.5	0.7	0.7
C_2H_4	-	0.3	-	0.1
	100.0	100.0	100.0	100.0
Gas heating value excluding H_2S Btu/SCF	239.	291.	290.	285.
No. of moles/ton of coal	212.6	160.6	158.	187.
Efficiency %				
Heating value of gas/ heating value of coal	79.9	77.5	75.8	75.3
Heating value of gas/ (Heating value of coal gasified + coal used for production of steam and power required)	58.7	52.8	50.9	48.8

Based on above datum level, the corresponding work equivalent of the chemical elements are calculated and are shown in Table 3.

Table 3 Available Work of Chemical Elements

Substance	State	ε at 25°C & 1 atm. Btu/mole
Coal*	Solid	224,460 (Btu/mole-C)
C	Solid	168,000'
S	Solid	127,560
O_2	Gas	1,670
N_2	Gas	250
H_2	Gas	101,210
H_2O	Gas	3,700
CO	Gas	109,780
CO_2	Gas	0
CH_4	Gas	348,570

*Pittsburgh seam coal is used. Entropy of coal is about 4 cal/gmole-carbon °K.

Energy utilization efficiency based on available work and percentage distribution of irreversibility for different process steps of Lurgi, Koppers-Totzek and Hydrane Processes were calculated. The results are shown in Table 4.

Table 4 Evaluation of irreversible work distribution in the coal gasification processes to produce pipeline gas.

(Feed Coal = 1 ton basis, Pittsburgh seam)

	Lurgi-Gasifier	Koppers-Totzek Gasifier	Hydrane Process
Feed coal, available work x 10^6 Btu	25.74	25.74	25.74
Product pipeline gas, available work x 10^6 Btu	15.30	13.49	16.72
Irreversible lost work x 10^6 Btu	10.44	12.25	9.02
Thermal eff.	64%	54%	72%
Available work eff.	59%	52%	65%
Irreversible lost work distribution, x 10^6 Btu			
Gasifier	3.82	4.03	4.16
Heat exchanger and spray tower	0.96	1.06	0.81
Shift converter	0.33	1.41	0.30
Purification unit	1.16	1.28	1.05
Methanation unit	1.09	1.80	0.13
Oxygen plant	1.34	2.06	0.86
Steam and power plant	1.74	0.61	1.71

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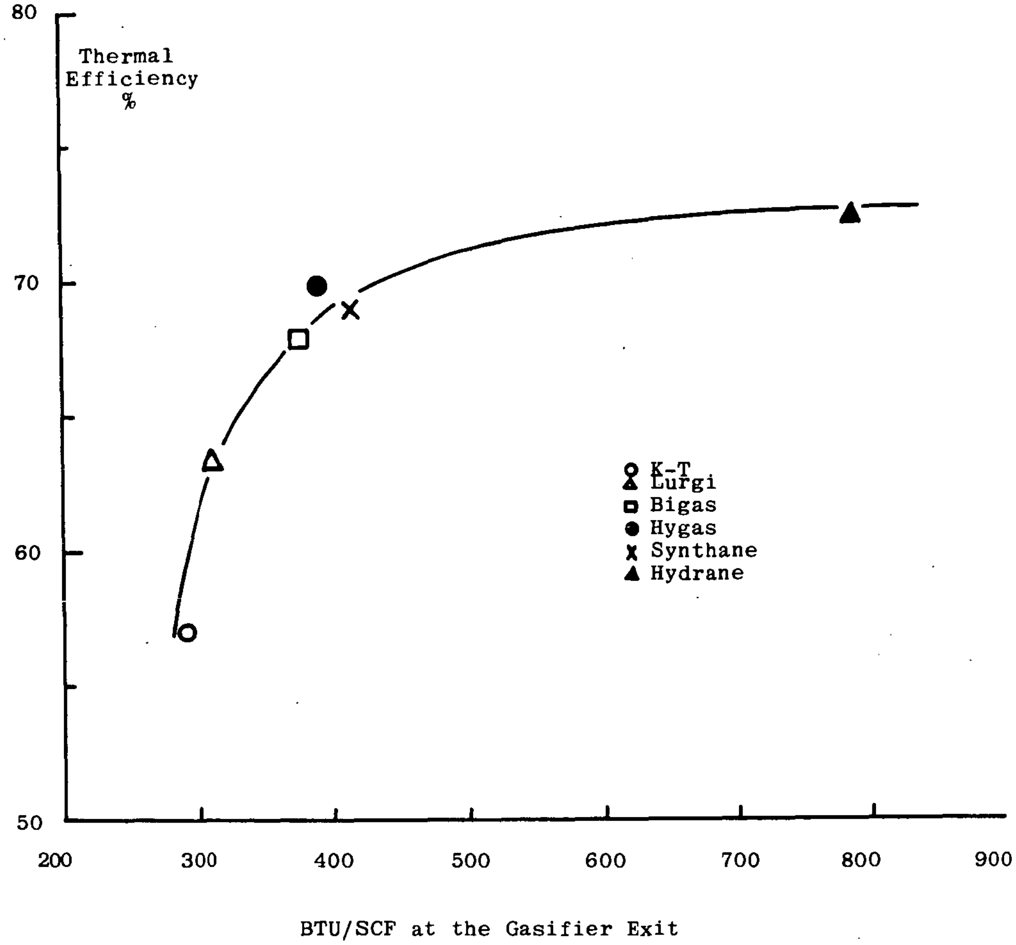

Figure 1 Effect of Amount of Methane Produced in the Gasifier on the Thermal Efficiency of the Process.